AR201-13955B

IUCLID

Data Set

New Chemical	:	ID: 126-86-3
CAS No.	:	126-86-3
EINECS Name	:	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
EINECS No.	:	204-809-1
Structural Formula	:	CC(CC(O)(C)C#CC(C)(CC(C)C)O)C

Producer Related Part

Company	:	Air Products and Chemicals, Inc.
Creation date	:	20.09.1999

Substance Related Part

Company	:	Air Products and Chemicals, Inc.
Creation date	:	20.09.1999
Memo	:	
Printing date	:	19.08.2002
Revision date	:	
Date of last Update	:	26.07.2002
Number of Pages	:	32
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic
Physical status : solid
Purity : >= 98 % w/w
20.09.1999

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1,4-Diisobutyl-1,4-dimethylbutynediol
20.09.1999

2,4,7,9-Tetramethyl-5-decyne-4,7-diol (ENCS, ECL)
20.09.1999

2,4,7,9-Tetramethyldec-5-in-4,7-diol (German) (EINECS)
20.09.1999

2,4,7,9-Tetramethyldec-5-yne-4,7-diol (English, French) (DSL, EINECS)
20.09.1999

5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- (TSCA, DSL, AICS)
20.09.1999

Surfynol 104
20.09.1999

1.3 IMPURITIES

CAS-No : 7732-18-5
EINECS-No :
EINECS-Name : Water
Contents : <= 2 % w/w

20.09.1999

CAS-No : 108-10-1
EINECS-No : 203-550-1
EINECS-Name : 4-methylpentane-2-one
Contents : <= 0.54 % w/w
13.12.2001

CAS-No :
EINECS-No :
EINECS-Name : Dimethyl Hexynol
Contents : <= 0.54 % w/w
13.12.2001

1.4 ADDITIVES

1.5 QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

1.7.1 TECHNOLOGY PRODUCTION/USE

Type : Use
Remark : Uses of 2,4,7,9-tetramethyl-5-decyne-4,7-diol

There are two major direct uses for 2,4,7,9-tetramethyl-5-decyne-4,7-diol (CAS # 126-86-3). Most of the 2,4,7,9-tetramethyl-5-decyne-4,7-diol manufactured is used as an industrial defoaming, nonionic surfactant. A lesser quantity of the product is consumed as a chemical intermediate and is converted into a polyethylene glycol ether surfactant, also for use in industrial applications.

2,4,7,9-tetramethyl-5-decyne-4,7-diol has been marketed for predominantly waterborne industrial applications in the coatings, ink, and adhesive industries. Though a critical contributor to the performance of a formulated product, the surfactant is generally applied in low use levels, typically 0.1 - 0.5%.

Due to its ability to reduce surface tension under dynamic conditions, 2,4,7,9-tetramethyl-5-decyne-4,7-diol surfactant is used to enhance wetting of oily or improperly cleaned substrates and to improve coverage over low surface tension substrates like plastic in waterborne architectural, industrial

surface tension substrates like plastic in waterborne architectural, industrial maintenance, general industrial, wood, plastic, concrete and paper coatings.

The 2,4,7,9-tetramethyl-5-decyne-4,7-diol surfactant is also employed for its multifunctional benefits in water-based printing inks. The product aids in penetration of the ink into absorbent stocks such as paper and also improves coverage over polymeric films such as polyethylene. In addition, the surfactant's unique capabilities eliminate foam, which causes many problems in printing inks. In overprint varnish systems, the surfactant provides wetting so that proper coverage of an aqueous overprint varnish can be achieved over wet solvent-based lithographic ink. The surfactant is also used in lithographic fountain solutions for the dynamic wetting of printing plates without causing excess emulsification of the ink. In pigment grinding applications, the surfactant provides good color development for maximum tint strength and lower viscosity dispersions for efficient grinding at higher pigment loadings.

2,4,7,9-tetramethyl-5-decyne-4,7-diol is used as a component of pressure sensitive adhesives, plywood adhesives, and laminating adhesives. The low surface tensions presented by silicone and plastic film release liners require strong wetting agents in order to achieve proper coverage by the adhesive.

The unique multifunctional properties of 2,4,7,9-tetramethyl-5-decyne-4,7-diol surfactant that make it successful in waterborne coatings, ink, and adhesive formulations also apply to several other applications. The following represent some of the other areas where our products are also used: industrial cleaners, agriculture, latex dipping, emulsion polymerization, foundry, metalworking fluids, and chemical processing.

In its other major use, some of the 2,4,7,9-tetramethyl-5-decyne-4,7-diol manufactured is converted to polyethylene glycol ether surfactants. These products represent a range of ethoxylation with varying water solubility, foaming and wetting characteristics.

13.12.2001

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.9 SOURCE OF EXPOSURE

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value	:	= 54 - 55 ° C
Decomposition	:	no
Sublimation	:	no
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	1999
GLP	:	yes
Test substance	:	

15.11.1999 (20)

2.2 BOILING POINT

Value	:	= 262 - 263 ° C
Decomposition	:	no
Method	:	OECD Guide-line 103 "Boiling Point/boiling Range"
Year	:	1999
GLP	:	yes
Test substance	:	
Remark	:	The measured boiling temperature depends on the atmospheric pressure. The determination of the correction factor to standard pressure is beyond the scope of this study. Therefore no correction was applied to the boiling temperature observed.

15.11.1999 (21)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 0.0062 - 0.007 hPa at 20° C
Decomposition	:	
Method		OECD Guide-line 104 "Vapour Pressure Curve"
Year	:	1999
GLP	:	yes
Test substance	:	

13.12.2001 (22)

2.5 PARTITION COEFFICIENT

Log pow	:	= 2.8 at 22° C
Method		OECD Guide-line 117 "Partition Coefficient (n-octanol/water), HPLC Method"
Year	:	1999

GLP : yes
Test substance :
16.12.1999 (23)

2.6.1 WATER SOLUBILITY

Value : = 1.7 g/l at 20 ° C
Qualitative : soluble (1000-10000 mg/L)
Pka :
PH : = 7.3 - 7.5
Method : OECD Guide-line 105 "Water Solubility"
Year : 1999
GLP : yes
Test substance :
16.12.1999 (24)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

INDIRECT PHOTOLYSIS

Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000424862 cm³/(molecule*sec)
Degradation	:	= 50 % after 3.021 hour(s)
Deg. product	:	
Method	:	other (calculated) using EPIWIN Suite (QSAR) Properties AOP Program (v1.90)
Year	:	2002
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	AOP Program (v1.90) Results: ========== SMILES : OC(C#CC(O)(CC(C)C)C)(CC(C)C)C CHEM : 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl- MOL FOR: C14 H26 O2 MOL WT : 226.36 ---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 15.2062 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec Addition to Triple Bonds = 27.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 42.4862 E-12 cm3/molecule-sec HALF-LIFE = 0.252 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 3.021 Hrs ---------- SUMMARY (AOP v1.90): OZONE REACTION ---------- OVERALL OZONE Rate Constant = 0.003000 E-17 cm3/molecule-sec HALF-LIFE = 382.000 Days (at 7E11 mol/cm3)
Remark	:	Photodegrades rapidly in the atmosphere.

15.03.2000 (17)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	
t1/2 pH7	:	
t1/2 pH9	:	
Deg. Product	:	
Method	:	OECD Guide-line 111 "Hydrolysis as a Function of pH"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Half-life time at 25 degrees C greater than 1 year at pH 4, pH 7, and pH 9.
Reliability	:	(1) valid without restriction

15.03.2000 (1)

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type :
Media :
Air (level I) :
Water (level I) :
Soil (level I) :
Biota (level II / III) :
Soil (level II / III) :
Method : other
Year : 2000
Method : EPIWIN Suite (QSAR) Properties.
STP Fugacity Model; predicted fate in a wastewater treatment facility.
Result : Molecular weight (g/mol) 226.36
Aqueous solubility (mg/l) 1700
Vapour pressure (Pa) 0.65328
(atm) 6.44737E-006
(mm Hg) 0.0049
Henry 's law constant (Atm-m3/mol) 8.58483E-007
Air-water partition coefficient 3.51094E-005
Octanol-water partition coefficient (Kow) 630.957
Log Kow 2.8
Biomass to water partition coefficient 126.991
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	2025.41	10000.00
-Aeration tank	0.00	2025.41	10000.00
-Settling tank	0.00	2025.41	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	4.4E-002	100.00
Primary sludge	1.72E-001	7.6E-004	1.72
Waste sludge	2.47E-001	1.1E-003	2.47
Primary volatilization	4.55E-004	2.0E-006	0.00
Settling volatilization	1.24E-003	5.5E-006	0.01
Aeration off gas	3.06E-003	1.4E-005	0.03
Primary biodegradation	2.15E-003	9.5E-006	0.02

Settling biodegradation	6.41E-004	2.8E-006	0.01
Aeration biodegradation	8.44E-003	3.7E-005	0.08
Final water effluent	9.56E+000	4.2E-002	95.65
Total removal	4.35E-001	1.9E-003	4.35
Total biodegradation	1.12E-002	5.0E-005	0.11

15.03.2000 (13)

Type :
Media :
Air (level I) :
Water (level I) :
Soil (level I) :
Biota (level II / III) :
Soil (level II / III) :
Method : other
Year : 2001
Method : EPIWIN V3.05 LEV3EPI Fugacity Model
Result : Level III Fugacity Model (Full-Output):

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Chem Name : 5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-
Molecular Wt: 226.36
Henry's LC : 8.58e-007 atm-m3/mole (calc VP/Wsol)
Vapor Press : 0.0049 mm Hg (user-entered)
Liquid VP : 0.00959 mm Hg (super-cooled)
Melting Pt. : 54.5 deg C (user-entered)
Log Kow : 2.8 (user-entered)
Soil Koc : 259 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.425	6.04	1000
Water	31.8	900	1000
Soil	67.4	900	1000
Sediment	0.383	3.6e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	8.53e-012	907	79.1	30.2	2.64
Water	1.12e-011	456	592	15.2	19.7
Soil	4.05e-011	964	0	32.1	0
Sediment	9.37e-012	1.37	0.142	0.0457	0.00475

Persistence Time: 620 hr
Reaction Time: 798 hr
Advection Time: 2.77e+003 hr
Percent Reacted: 77.6
Percent Advected: 22.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 6.039
Water: 900
Soil: 900
Sediment: 3600

Sediment: 3600
Biowin estimate: 2.275 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

13.12.2001

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	
Degradation	:	= 5% after 28 day
Result	:	
Deg. Product	:	
Method	:	OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year	:	1999
GLP	:	Yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was tested for its ready biodegradability in the carbon dioxide (CO2) evolution test (modified Sturm test) at 36.3 ml per 2 litres, corresponding with 12 mg TOC/l. The Theoretical CO2 production (ThCO2) of 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was calculated to be 2.72 mg CO2/mg, corresponding with 2.42 mg CO2/ml. The relative degradation values calculated from the measurements performed during the test period revealed no significant degradation of 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol. In the toxicity control, 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was found not to be inhibitory.
Reliability	:	(1) valid without restriction

15.03.2000 (14)

Type	:	aerobic
Inoculum	:	activated sludge, domestic
Contact time	:	57 days
Degradation	:	= 25.4 % daily during the last 16 days of study
Result	:	15.7 % (57 day daily average)
Conclusion	:	Inherently biodegradable
Deg. Product	:	
Method	:	OECD Guide-line 302 A “Inherent Biodegradability: Modified Semi-Continuous Activated Sludge (SCAS) test“

Year	:	1999
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The test was run at 20-25 degrees C under low light conditions. The test volume was 1500 mL total. The renewal volume was 1000 mL daily. 2 replicates were tested per treatment. 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was tested for its biodegradability in a Semi-Continuous Activated Sludge (SCAS) system at a daily dosage level starting at approximately 8-10 ppm as TOC, but later continued at an averagedosage level of 15 ppm. Less than 5% physical removal (abiotic absorption) was detected in an intra-test sludge treatment trial. In the toxicity control, 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was found not to be inhibitory. Aniline (positive control) degraded on average >95%, validating the test system.
Reliability	:	(1) valid without restriction

15.03.2000 (18)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	No
LC50	:	= 36
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	1991
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Fish measuring 2 cm +/- 1 cm at the start of test were exposed to Surfynol 104 at concentrations of 0, 4, 8, 16, 32, and 64 ppm. Two groups of 10 fish were exposed at each concentration. The dissolved oxygen, water pH, specific conductance, total hardness and total alkalinity were measured. All deaths occurred within the first 24 hours. Statistical analysis was performed using the Trimmed Spearman-Karber method. Information on fish age, and test temperature and lighting were not recorded.
Reliability	:	(2) valid with restrictions

06.11.2001 (4)

Type	:	static
Species	:	Cyprinus carpio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= 10
LC0	:	= 32
LC50	:	= 42
LC100	:	= 56
Method	:	OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

The batch of 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol tested was a 98.3 percent pure, white solidified mass and was completely soluble in test medium at the concentrations tested. Preparation of test solutions started with heating the test substance for approximately one hour in a water bath at 90 degrees C. The appearance of the substance changed to a clear yellow viscous liquid.

First a range-finding test was conducted with exposure of fish to 0.1, 1.0, 10 and 100 mg/l. All fish died at 100 mg/l within 2.5 hours after the start of the test, while no fish died at 10 mg/l. Analysis of samples taken at 10 mg/l showed that this concentration was stable during the 96-hour test period.

After the range-finding test, a final test was performed with carp exposed to concentrations of 0, 10, 18, 32, 56 and 100 mg/l in a static system. Seven carp were exposed per concentration and a control. The loading was 0.67 g fish/liter. At the start of test, the water hardness was 250 mg $CaCO_3$ per liter, the dissolved oxygen concentration was saturated, and the water pH was 8.0. The dissolved oxygen, water pH, and temperature were measured daily. Samples for analytical confirmation of actual exposure concentrations were taken at the start and the end of the test.

Analysis of the samples taken during the final test showed that the measured concentrations in the samples taken at the start of the test were 9.5 mg/l (95 percent), 28.3 mg/l (89 percent) and 88.6 mg/l (89 percent) at the nominal concentrations of 10, 32 and 100 mg/l, respectively. The measured concentrations at 32 and 100 mg/l could be related to lower recoveries found at 180 mg/l in a recovery control experiment (87-90 percent). Hence, the actual concentrations in these samples were considered to be in agreement with nominal. At the end of the test period measured concentrations had not decreased by more than 20 percent of the initial concentrations. As a result, toxicity parameters were based on nominal concentrations.

Results : The test temperature ranged from 20.2 to 20.8 degrees C. The pH ranged from 8.1 to 7.5 and the dissolved oxygen was within the prescribed range.

The 24h- and 96h-LC50 for carp exposed to 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was 42 mg/l with 0 percent mortality at 32 mg/l (LC0) and 100 percent mortality at 56 mg/l (LC100). Concentrations down to 18 mg/l induced effects on swimming behavior and pigmentation, while no sub-lethal effects occurred at 10 mg/l.

Reliability : (1) valid without restriction
14.06.2001 (11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
EC50	:	= 88
Method	:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year	:	1991

GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Daphnia which were < 27 hours old at the start of test were exposed to Surfynol 104 at concentrations of 0, 62.5, 125, 250, 500, and 1000 ppm. Four groups of 5 daphnia were exposed at each concentration. The dissolved oxygen, water pH, specific conductance, total hardness and total alkalinity were measured. Statistical analysis was performed using the Trimmed Spearman-Karber method. Information on test temperature and lighting were not recorded.
Reliability	:	(2) valid with restrictions

06.11.2001 (4)

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= 43
EC50	:	= 91
Method	:	OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4 The batch of 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol tested was a 98.3 percent pure, white solidified mass and was completely soluble in test medium at the concentrations tested. Preparation of test solutions started with heating the test substance for approximately one hour in a water bath at 90 degrees C. The appearance of the substance changed to a clear yellow viscous liquid. First a range-finding test was conducted exposing 10 daphnia per vessel to concentrations ranging from 0.001 to 100 mg/l. At the end of the 48-hour test period 4 out of 10 daphnids exposed to 100 mg/l became immobilized. Based on the results of the range-finding test a final EC50 test was performed exposing Daphnia for a maximum of 48 hours to nominal concentrations of 0, 18, 32, 45, 100, and 180 mg/l. The test was performed in duplicate with 10 daphnia per vessel. Samples for determination of actual exposure concentrations were taken at the start and the end of the final test. Analysis of samples taken during the final study showed that the average exposure concentrations at the concentrations essential for determination of the toxicity parameters, i.e. 56, 100, and 180 mg/l, were 42.5, 84.2, and 165 mg/l, respectively. The 48h-EC50 for Daphnia magna exposed to 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol was 91 mg/l based on average exposure concentrations with a 95 percent confidence interval between 81 and 110 mg/l. The 24h-EC50 was 99 mg/l with a 95 percent confidence interval between 83 and 130 mg/l. 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol did not induce acute immobilization of Daphnia magna at 43 mg/l after 48 hours of exposure (NOEC).

Reliability : (1) valid without restriction
14.06.2001 (10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
NOEC	:	= 1
EC10	:	= 1.8
EC50	:	= 15
Method	:	OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year	:	2000
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4 The batch of 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol tested was a 98.3 percent pure, white solidified mass and was completely soluble in test medium at the concentrations tested. Preparation of test solutions started with heating the test substance for approximately one hour in a water bath at 90 degrees C. The appearance of the test substance changed to a clear yellow viscous liquid. After a range-finding test, a final test was performed exposing exponentially growing algal cultures to 2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol concentrations ranging from 1 to 100 mg/l, increasing with a factor of 2.2. The initial cell density was 104 cells/ml. The total test period was 72 hours. Samples for analysis were taken at 1.0, 10 and 100 mg/l at the start and the end of the test. Measured concentrations were greater than 100 percent of nominal in all samples analysed. Based on a recovery experiment simultaneously performed, the measured values indicated that the actual concentrations were in agreement with nominal and remained stable during the test period.
Result	:	2,4,7,9-Tetramethyl-5-Decyne-4,7-Diol affected growth of the fresh water algae species Selenastrum capricornutum significantly at 2.2 mg/l and higher. The NOEC for cell growth inhibition and growth rate reduction was 1.0 mg/l. However, a recovery of growth was observed during the last 48 hours of exposure with a NOEC of 4.6 mg/l for growth rate. The EC50 for cell growth inhibition (EBC50: 0-72h) was 15 mg/l with a 95 percent confidence interval ranging from 9 to 23 mg/l. The EC10 for cell growth inhibition (EBC10: 0-72h) was 1.8 mg/l with a 95 percent confidence interval ranging from 1.1 to 3.0 mg/l. A more time related response appeared by comparison of the reduction of growth rate for different time intervals. Cell growth rate reduction: EC10 (0-72h) equal to 15 mg/l (95% confidence limits 7 to 30);

EC50 (0-72h) equal to 82 mg/l (95% confidence limits 39 to 170).

Cell growth rate reduction:
EC10 (24-72h) equal to 15 mg/l (95% confidence limits 7 to 31);
EC50 (24-72h) equal to 39 mg/l (95% confidence limits 19 to 81).

Reliability : (1) valid without restriction
15.03.2000 (12)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : activated sludge
Exposure period : 30 minute(s)
Unit : ppm
Method : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year : 1999
GLP : Yes
Test substance : as prescribed by 1.1 - 1.4
Method : 2,4,7,9-tetramethyl-5-decyne-4,7-diol was tested at 12, 37, 111, 333, and 1000 ppm w/v. The test was run at 20 ° C. 2,4,7,9-tetramethyl-5-decyne-4,7-diol was soluble in warm water at just below 1000 ppm so at the test temperature some test material remained undissolved. 3,5-dichlorophenol was run as a positive control.
EC50 were calculated from EPA „Probit Analysis for Calculating LC/EC Values, version 1.5“
Result : The maximum concentration of the test material that proved without inhibition was 111 ppm. The 30-minute EC50 was estimated as 630 ppm.
The EC50 of 3,5-dichlorophenol was estimated as 14.5 ppm (CI= 8.3-25.3).
Reliability : (2) valid with restrictions
07.03.2002 (18)

Type : aquatic
Species : activated sludge
Exposure period : 3 hour(s)
Unit : ppm
Method : OECD Guide-line 209 "Activated Sludge, Respiration Inhibition Test"
Year : 1999
GLP : Yes
Test substance : as prescribed by 1.1 - 1.4
Method : 2,4,7,9-tetramethyl-5-decyne-4,7-diol was tested at 12, 37, 111, 333, and 1000 ppm w/v. The test was run at 20 ° C. 2,4,7,9-tetramethyl-5-decyne-4,7-diol was soluble in warm water at just below 1000 ppm so at the test temperature some test material remained undissolved. 3,5-dichlorophenol was run as a positive control.
EC50 were calculated from EPA „Probit Analysis for Calculating LC/EC Values, version 1.5“
Result : The maximum concentration of the test material that proved without inhibition was 111 ppm. The 3-hour EC50 was estimated as 840 ppm (CI= 744-963).
The EC50 of 3,5-dichlorophenol was estimated as 5.6 ppm.
Reliability : (2) valid with restrictions
07.03.2002 (18)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other
Value	:	> 500 mg/kg bw
Method	:	other
Year	:	1971
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	5 male and 5 female Sprague-Dawley rats with an average body weight of 191 grams were fasted for approximately 18 hours prior to dosing. The Surfynol 104 was prepared as a 5% solution in hydrous alcohol. Each rat received a dose volume of 10 ml/kg of body weight. The animals were observed daily post-dose for 14 days.
Result	:	All animals survived, showed no abnormal clinical signs and gained weight. Gross necropsy did not reveal any test material-related pathological changes.
Reliability	:	(2) valid with restrictions Study pre-dates GLPs.

13.12.2001 (3)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	rat
Strain	:	
Sex	:	male/female
Number of animals	:	10
Vehicle	:	water
Exposure time	:	1 hour(s)
Value	:	> 20 mg/l
Method	:	other
Year	:	1971
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	5 male rats (average weight 176 grams) and 5 female rats (average weight 211 grams) were placed in a 306 liter chamber. The Surfynol 104 was prepared as a 5% aqueous solution. An air flow of five liters per minute was introduced into the chamber. The test solution was aerosolized to provide a concentration of greater than 20 mg of mist per liter of chamber air over the one-hour period. The test atmosphere was not analyzed. The animals were observed daily for 14 days.
Result	:	All animals survived. Ocular and nasal irritation as well as a reduction in spontaneous activity was noted in all animals immediately following the one-hour exposure. All animals returned to normal within 3 hours. One male and one female were autopsied at random. Gross necropsy did not reveal any test material-related pathological changes.

Reliability	:	(2) valid with restrictions Study pre-dates GLPs

13.12.2001 (3)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	:	> 2000 mg/kg bw
Method	:	OECD Guide-line 402 "Acute dermal Toxicity"
Year	:	1993
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Test substance	:	Surfynol 104 batch # 21902
Reliability	:	(1) valid without restriction

21.09.1999 (6)

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	no data
Number of animals	:	6
Vehicle	:	
Value	:	> 1000 mg/kg bw
Method	:	other
Year	:	1971
GLP	:	
Test substance	:	
Method	:	6 New Zealand White rabbits with an average body weight of 3 kilograms were selected for dosing. The skin of the trunk was clipped free of hair exposing an average surface area of approx. 240 square centimeters. The neat Surfynol 104 (1000 mg/kg) was applied to the intact skin site. The entire trunk of each animal was then encased in a plastic sleeve to insure continuous contact of the test material with the skin for a 24-hour period. The sleeve was removed after 24-hours and the animals were observed daily post-dose for 14 days.
Test substance	:	Surfynol 104 was applied neat.
Reliability	:	(2) valid with restrictions

06.11.2001 (3)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	Semiocclusive

Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	
Result	:	
EC classification	:	irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1993
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Moderate to severe erythema and slight edema in the animals. Reduced flexibility of the treated skin was noted in two animals 72 hours after exposure only. The skin irritation had resolved within 21 days after exposure in all animals. No corrosive effect occurred on the skin in any of the three rabbits. Primary irritation index of 4.3 (moderately irritating) when melted and applied to the intact skin.
Reliability	:	(1) valid without restriction

06.11.2001 (5)

Species	:	rabbit
Concentration	:	
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	3
PDII	:	
Result	:	slightly irritating
EC classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1994
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The test article was weighed and 0.5 g was moistened with distilled water (made pasty) to ensure good contact with the skin. The resultant paste was applied to the clipped site in a manner allowing even distribution of the test article over the 6 centimeter squared test site. The test site was then covered with a semiocclusive dressing.
Result	:	Erythema, slight at 30 - 60 minutes after patch removal, was absent to slight at 24 hours and absent at 48 and 72 hours. Edema, was absent at all observation intervals. There were no abnormal physical signs noted during the observation period. Primary Irritation Index of 0.17 (mildly irritating) when applied to the intact skin as a paste.

13.12.2001 (19)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	0.1 ml
Exposure Time	:	
Comment	:	
Number of animals	:	9

Result	:	highly irritating
EC classification	:	irritating
Method	:	other
Year	:	1998
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	EPA/TSCA Health Effects Testing Guidelines, 40 CFR Part 798.45.00.
Remark	:	Nine healthy New Zealand White rabbits, free from evidence of ocular irritation and corneal abnormalities, were dosed. Surfynol 104 (0.1 ml) was placed into the conjunctival sac of one eye of each rabbit. Six eyes remained unwashed. Three eyes were washed with lukewarm water for one minute, 30 seconds postdose. The eyes were examined and scored by the Draize technique at one hour and at 24, 48, and 72 hours postdose. In order to determine reversibility, the eyes were examined again on Days 7, 14, and 21. Sodium fluorescein was used to determine corneal effects following the 24-hour scoring interval.
Result	:	Unwashed eyes: Corneal opacity, noted in 6/6 eyes, persisted to Day 21 in 3/6 eyes. Iritis, noted in 6/6 eyes, cleared by Day 7. Conjunctival irritation, noted in 6/6 eyes, cleared by Day 14. Washed eyes: Corneal opacity, noted in 3/3 eyes, cleared by Day 14. Iritis, noted in 3/3 eyes, cleared by Day 7. Conjunctival irritation, noted in 3/3 eyes, cleared by Day 14.
Reliability	:	(1) valid without restriction

21.09.1999 (9)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	male/female
Strain	:	Long-Evans
Route of admin.	:	oral feed
Exposure period	:	28 days
Frequency of treatment	:	continuous
Post obs. period	:	
Doses	:	0, 625, 1250, 2500, and 5000 ppm
Control group	:	yes, concurrent no treatment
NOAEL	:	= 5000 ppm
Method	:	other
Year	:	1977
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Rats were assigned to groups by body weight. Each group was composed of 6 rats of each sex. The rats were approximately 6-7 weeks of age at the start of the test. Test diets were made up on a weekly basis. Statistical analysis of the body weight and food consumption data was performed using the F-test and the Student's t-test.
Result	:	Mortality, physical observations, body weight, and food consumption data, as well as gross necropsy observations did not reveal any adverse effects

as well as gross necropsy observations did not reveal any adverse effects considered to be attributable to the administration of Surfynol 104 at any of the dose levels. NOEL=5000 ppm (high-dose).

Reliability : (2) valid with restrictions
Study pre-dates GLPs

21.09.1999 (2)

Species	:	dog
Sex	:	male/female
Strain	:	Beagle
Route of admin.	:	other
Exposure period	:	130 days
Frequency of treatment	:	daily
Post obs. period	:	
Doses	:	0, 200, 250, and 300 mg/kg/day
Control group	:	yes
LOAEL	:	= 200 mg/kg
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : 32 pure-bred Beagles (16 of each sex) weighing approx. 4.6 to 9.0 Kg and being 4-5 months of age were quarantined for 21 days and then randomized into four groups each containing 4 males and 4 females. Randomization was performed in such a way that no same sex siblings were in the same group and an even distribution of body weights was obtained. All groups received 350 grams of food per day. All dosing was done using ¼ ounce gelatin capsules. Capsule administration followed feeding by approximately one hour. The control animals received capsules of granulated table sugar. The low-dose group received 50 to 200 mg of Surfynol 104 per kg of body weight per day. The mid- and high-dose group received 50 to 300 mg/kg/day. The mean weekly body weight of each group was used to calculate the dose. Doses were calculated separately for each sex. Statistical analysis of the body weight, food consumption, clinical chemistry, hematology and organ weight data was performed using the Student t test.

Remark : The test material was administered orally to beagle dogs in gelatin capsules at dose levels of 200, 250 and 300 mg/kg/day for 91 days. Because the dogs had to be gradually acclimated from 50 mg/kg/day to higher dose levels of SURFYNOL 104 to avoid vomiting, the total test period was 130 days.

Result : All dogs survived for the duration of this study with few clinical signs. Occasional dogs in the mid- and high-dose groups exhibited sporadic compound-related neurologic disturbances (convulsions and tremors) during the study. All other observations, including feed consumption, body weight gains, organ weights (except liver), clinical chemistries, hematology, urinalysis, gross pathology, and histology were judged to reflect no compound-related/ biologically significant changes. This study did not establish a no-effect level (NOEL) of Surfynol 104 in dogs, since mean liver weights and liver-to-body weight ratios in all Surfynol 104-treated groups were higher than in corresponding control groups. However, since no historical abnormalities were observed in these livers, the liver enlargement was judged to be due to hyperplasia of the hepatic endoplasmic reticulum, where xenobiotic/drug metabolizing enzymes are located. These common

where xenobiotic/drug metabolizing enzymes are located. These common adaptive liver changes are generally reversible, after test compound exposure is discontinued.

Test substance : Surfynol 104 lot # 2910-109 (purity 100%)
Reliability : (2) valid with restrictions
13.12.2001 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium strains TA1535, TA1537, TA98, TA100, and E-coli strain WP2(uvrA).
Concentration : 0, 10, 50, 100, 500, 1000, and 5000 ug/plate
Cycotoxic conc. : 1000
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1999
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : 2,4,7,9-tetramethyl-5-decyne-4,7-diol diluted in DMSO was examined for mutagenic activity in the Salmonella-Escherichia coli/microsome plate incorporation assay. The assay was performed using the standard plate incorporation procedure with S. typhimurium strains TA1535, TA1537, TA98, and TA100 and E. coli strain WP2 (uvrA) over a dose range of 10 to 5000 ug/plate in both the presence and absence of an Aroclor 1254-induced rat-liver metabolic activation system. The initial experiment used 5 percent (v/v) metabolic activation and the repeat experiment used 10 percent (v/v) metabolic activation.
Result : The 5000 ug/plate dose formulation appeared to be immiscible in the tubes and on the plates. Precipitate was also observed in the tubes and on the plates at a dose level of 5000 ug. However after the 48-hour incubation period the precipitate was no longer seen on the plates. Cytotoxicity, indicated by thinning of the background bacterial lawn and the formation of pinpoint nonrevertant colonies, was observed for all strains generally at dose levels of 1000 and 5000 ug/plate.

No 2,4,7,9-tetramethyl-5-decyne-4,7-diol treatments of the test strains resulted in an increase in revertant numbers that was considered indicative of any mutagenic activity.
Reliability : (1) valid without restriction
15.03.2000 (15)

Type : Cytogenetic assay
System of testing : CHO Cells
Concentration : 19.5, 39.1, 78.1-78.3, 156.3, 312.5, 1250, and 3500 ug/ml
Cycotoxic conc. : 312.5
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473 "Genetic Toxicology: In vitro Mammalian Cytogenetic Test"
Year : 1999

GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	In the cytotoxicity assay, CHO cells were exposed to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at concentrations of 19.5, 78.3, 312.5, 1250, and 3500 ug/mL in both the absence and presence of MA. A high dose of 3500 ug/mL was used based on the limit of solubility of the test article in dimethylsulfoxide (DMSO). Cells were exposed to the test article in the absence of MA for 3 and 21 hr and in the presence of MA for 3 hr. At 21 hr after exposure initiation, cells were harvested and evaluated. Based on the cytotoxicity results, the initial chromosome aberration study was performed by exposing CHO cells for 3 hr to 2,4,7,9-tetramethyl-5-decyne-4,7-diol at concentrations of 19.5, 39.1, 78.1, 156.3, and 312.5 ug/mL in both the absence and presence of MA. At 21 hr after initiation of exposure, cells were harvested and evaluated. The dose levels for the replicate experiment were based on the results of the cytotoxicity experiment (-MA) and the initial experiment (+MA). The replicate experiment was performed by exposing CHO cells for 21 hr to the test article at concentrations of 9.8, 19.5, 39.1, 78.1, and 156.3 ug/mL in the absence of MA and for 3 hr at concentrations of 19.5, 39.1, 78.1, and 156.3 ug/mL in the presence of MA. At 21 hr after initiation of exposure, cells were harvested and evaluated.
Results	:	In the cytotoxicity experiment, all of the cultures from the top two dose levels exhibited a significant decrease in confluency (0 to 25 percent) and therefore were not harvested. For cultures exposed to the test article for 3 hr in the presence or absence of MA, no significant reduction in mitotic index was observed at dose levels of 312.5 ug/mL and below. Cultures exposed for 21 hr to the test article at 312.5 ug/mL showed a significant reduction in mitotic index. In the initial chromosome aberration experiment, cytotoxicity was evident in cultures exposed to 312.5 ug/mL under both MA conditions, so the cells were not harvested for evaluation. In both the initial chromosome aberration experiment and in the replicate experiment, there was no statistically significant increase in the number of cells with structural aberrations at the three dose levels scored in both MA conditions (39.1, 78.1, and 156.3 ug/mL). The mitotic index was comparable to that for the control and no increases in polyploidy were observed in the presence or absence of MA.
Reliability	:	(1) valid without restriction

15.03.2000 (16)

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

5.8 TOXICITY TO REPRODUCTION

Type	:	One generation study
Species	:	rat

Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	variable
Frequency of treatment	:	continuous
Premating exposure period		
Male	:	None
Female	:	None
Duration of test	:	135 days
Doses	:	0, 500, 1000, and 2000 mg/kg/day
Control group	:	yes, concurrent no treatment
NOAEL Parental	:	= 500 mg/kg bw
NOAEL F1 Offspr.	:	= 500 mg/kg bw
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Ten male and twenty female sexually mature rats were randomly assigned to each group. Males were sacrificed following the 20th day of breeding and females were sacrificed when their litters were weaned at 21 days of age. Animals were fed their respective diets from the start of cohabitation until their scheduled sacrifice. The weanlings were randomized within their respective groups and carried on the same dose levels as their parents for 91 days. Test diets were prepared weekly. Analytical monitoring of the test diets was performed. Statistical analysis of the body weight, food consumption, clinical chemistry, and hematology data was performed using the Student's t-test.
Result	:	The only pertinent findings observed in the Fo parents were: a slight decrease in the mean weaning weight of both male and female pups of the high-dose group, a slight decrease in lactation indices of the high-dose group, decreased body weight and feed consumption of the high-dose female group and normal histology of the reproductive organs in the Fo parents. Fertility, viability and gestation indices were not affected. In the reproduction phase of this experiment there was a toxic effect at the 2,000 mg/kg/day level, a borderline effect at the 1,000 mg/kg/day level and no effect at 500 mg/kg/day.

Surfynol 104: Summary of F0/F1a Reproduction Data

Dose Group	Number of Dams		Total Number of Pups				
(mg/kg/day)	Mated	Conceived	Live-born	Still-born	Day 4	Culled Day 4*	Day 21
0	20	20	235	4	226	43	180
500	20	20	252	2	247	51	195
1000	20	20	229	0	220	37	173
2000	20	19	225	4	214	27	164

* Litters with more than 10 pups were culled to 10

Surfynol 104: Summary of F0/F1a Reproduction Data (continued)

Dose Group	Avg. # of Pups/Litter				Avg. Pup Weaning Weight (g)	
(mg/kg/day)	Day 4 M	F	Weaned M	F	Male	Female
0	6.0	5.4	4.6	4.5	45.7	44.2
500	6.6	5.8	5.0	4.8	42.0	40.9
1000	5.8	5.3	4.6	4.1	36.6	35.8
2000	5.5	5.8	4.1	4.6	28.8	25.7

The following pertinent findings were observed in the F1a rats: slight decrease in the mean rate of body weight gain in both sexes at the mid- and high-dose (there was also a significant decrease in this parameter in the low-dose male group during the first eight weeks), normal mean hematological findings, clinical chemistry findings, and urinalysis findings after 91 days on test, significant increase in the absolute and relative liver weights of both sexes at the mid- and high-dose, corresponding histopathology of the liver showing mild to moderate centrilobular cloudy swelling of hepatocytes of the mid- and high-dose rats. Surfynol 104, when fed to rats under the conditions of this experiment, showed no effect at 500 mg/kg/day but did have a toxic effect in the F1a generation at >1,000 mg/kg/day.

Test substance : Surfynol 104 lot # 2910-109 (purity 100%)
Reliability : (1) valid without restriction
21.09.1999 (8)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Type : One generation study
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : variable
Frequency of treatment : continuous
Premating exposure period
Male : None
Female : None
Duration of test : 135 days
Doses : 0, 500, 1000, and 2000 mg/kg/day
Control group : yes, concurrent no treatment
NOAEL Parental : = 500 mg/kg bw
NOAEL F1 Offspr. : = 500 - mg/kg bw
Method : other
Year : 1979
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Method : Ten male and twenty female sexually mature rats were randomly assigned to each group. Males were sacrificed following the 20th day of breeding and females were sacrificed when their litters were weaned at 21 days of age. Animals were fed their respective diets from the start of cohabitation until their scheduled sacrifice. The weanlings were randomized within their

until their scheduled sacrifice. The weanlings were randomized within their respective groups and carried on the same dose levels as their parents for 91 days. Test diets were prepared weekly. Analytical monitoring of the test diets was performed. Statistical analysis of the body weight, food consumption, clinical chemistry, and hematology data was performed using the Student's t-test.

Result : The only pertinent findings observed in the Fo parents were: a slight decrease in the mean weaning weight of both male and female pups of the high-dose group, a slight decrease in lactation indices of the high-dose group, decreased body weight and feed consumption of the high-dose female group and normal histology of the reproductive organs in the Fo parents. Fertility, viability and gestation indices were not affected. In the reproduction phase of this experiment there was a toxic effect at the 2,000 mg/kg/day level, a borderline effect at the 1,000 mg/kg/day level and no effect at 500 mg/kg/day.

Surfynol 104: Summary of F0/F1a Reproduction Data

Dose Group	Number of Dams		Total Number of Pups				
(mg/kg/day)	Mated	Conceived	Live-born	Still-born	Day 4	Culled Day 4*	Day 21
0	20	20	235	4	226	43	180
500	20	20	252	2	247	51	195
1000	20	20	229	0	220	37	173
2000	20	19	225	4	214	27	164

* Litters with more than 10 pups were culled to 10

Surfynol 104: Summary of F0/F1a Reproduction Data (continued)

Dose Group	Avg. # of Pups/Litter				Avg. Pup Weaning Weight (g)	
(mg/kg/day)	Day 4 M	Day 4 F	Weaned M	Weaned F	Male	Female
0	6.0	5.4	4.6	4.5	45.7	44.2
500	6.6	5.8	5.0	4.8	42.0	40.9
1000	5.8	5.3	4.6	4.1	36.6	35.8
2000	5.5	5.8	4.1	4.6	28.8	25.7

The following pertinent findings were observed in the F1a rats: slight decrease in the mean rate of body weight gain in both sexes at the mid- and high-dose (there was also a significant decrease in this parameter in the low-dose male group during the first eight weeks), normal mean hematological findings, clinical chemistry findings, and urinalysis findings after 91 days on test, significant increase in the absolute and relative liver weights of both sexes at the mid- and high-dose, corresponding histopathology of the liver showing mild to moderate centrilobular cloudy swelling of hepatocytes of the mid- and high-dose rats. Surfynol 104, when fed to rats under the conditions of this experiment, showed no effect at 500 mg/kg/day but did have a toxic effect in the Fla generation at >1,000 mg/kg/day.

Test substance : Surfynol 104 lot # 2910-109 (purity 100%)

Reliability : (1) valid without restriction
21.09.1999 (8)

5.10 OTHER RELEVANT INFORMATION

5.11 EXPERIENCE WITH HUMAN EXPOSURE

(1) APCI (EXT-00/001) / NOTOX

(2) APCI (EXT-77/016) / Biodynamics, Inc.

(3) APCI (EXT-86/020) / Foster D. Snell Inc. Biological Science Laboratories

(4) APCI (EXT-92/040) / Commonwealth Technology, Inc.

(5) APCI (EXT-94/010) / NOTOX

(6) APCI (EXT-94/012) / Notox B.V.

(7) APCI (EXT-94/090) / Pharmacopathics Research Laboratories

(8) APCI (EXT-97/005) / Pharmacopathics Research Laboratories

(9) APCI (EXT-98/164) / MB Research

(10) APCI (EXT-99/101) / NOTOX

(11) APCI (EXT/00-007) / NOTOX

(12) APCI (EXT/00-030) / NOTOX

(13) APCI (EXT/00-059) / NOTOX

(14) APCI (EXT/99-007) / NOTOX

(15) APCI (EXT/99-078) / SRI International

(16) APCI (EXT/99-091) / SRI International

(17) EPIWIN v3.05

(18) APCI (PFT-99/004) / SGS U.S. Testing Company Inc.

(19) APCI (EXT-94/062) / MB Research

(20) APCI (EXT-99/084) / Notox B.V.

(21) APCI (EXT-99/083) / Notox B.V.

(22) APCI (EXT-99/082) / Notox B.V.

(23) APCI (EXT-99/100) / Notox B.V.

(24) APCI (EXT-99/099) / Notox B.V.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

Remark : Potential for Worker Exposure During 2,4,7,9-tetramethyl-5-decyne-4,7-diol Manufacturing

2,4,7,9-tetramethyl-5-decyne-4,7-diol is produced by the reaction of acetylene and ketone. The crude product stream is continuously extracted from the reactor and then batch distilled. Once final product is obtained from the distillation, the product is blended with solvents to make one of several liquid products, or converted to polyethylene glycol ether surfactants via ethoxylation. The products can be drummed, loaded into totes, or loaded into trailers for bulk customer shipments. Workers in the drumming operation, which is ventilated mechanically, wear personal protective equipment including gloves, coveralls, and eye protection.

Most 2,4,7,9-tetramethyl-5-decyne-4,7-diol sold for surfactant applications is provided to industrial users. Because the surfactant is a difficult-to-handle, waxy solid, nearly all of these users purchase the product in 55-gallon drums or bulk quantities dissolved in a suitable solvent. The solvent enables ready formulation into a coating, ink, or adhesive and minimizes worker contact with the surfactant itself. Workers who make inks, coatings, or adhesives generally transfer the surfactant into day tanks where it is subsequently delivered into mixing units without additional need for human intervention. Such formulated products contain very low levels of 2,4,7,9-tetramethyl-5-decyne-4,7-diol.

Risk Management

The known toxicity information about 2,4,7,9-tetramethyl-5-decyne-4,7-diol suggests the acute effects of greatest concern are skin and eye irritation. Personal protective equipment recommendations for these effects are believed to be sufficient to protect against low levels of dermal exposure as well. 2,4,7,9-tetramethyl-5-decyne-4,7-diol has a low vapor pressure and low acute inhalation toxicity so unusual ventilation requirements are not required.

Based on the known toxicological endpoints, the following personal protection / exposure controls are recommended:

Eye protection: Splash-proof eye goggles. In emergency situations, use eye goggles with a full-face shield.

Hand protection: Neoprene rubber gloves. Nitrile rubber gloves. Insulated gloves such as thermal lined rubber when handling hot material.

Ventilation: Well-ventilated workplace.

Protective clothing: Long sleeved clothing.

Work and hygienic practices: Provide readily accessible eye wash stations and safety showers. Wash at the end of each work shift and before eating, smoking or using the toilet.

13.12.2001